We investigate representing discrete scientific data with a piecewise-continuous functional model. The MFA—Multivariate Functional Approximation—model can be analytically evaluated and differentiated to high order anywhere in the domain, making it ideal for subsequent data analysis. Often, the MFA is smaller in size than the original data, offering compression as well. These capabilities—evaluation, differentiation, and compression—can potentially transform how scientific datasets are represented and analyzed.

### High-Dimensional Modeling

A Nonuniform rational B-spline (NURBS) curve as a function of a parameter \( u \), basis functions \( N \), and control points \( P \): 
\[
C(u) = \sum_{j=0}^{p} N_j(u)P_j,
\]

where \( N_j(u) \) are the basis functions and \( P_j \) are the control points.

### Multivariate Approximation

1. Given a set of multivariate data points \( (x_1, y_1, z_1, t_1, v_1, ..., y_n, z_n, t_n, v_n) \), where science variables \( (y_1, y_2, ..., y_n) \) are a function of space-time geometry \( (x, y, z, t) \).
2. Map the geometry domain to an independent set of domain parameters \( P: (x, y, z, t) \rightarrow (u_1, u_2, u_3, u_4) \).
3. Build separate MFA models for the geometry and for each science variable over the same set of parameters. Models have independent degree, knots, and control points.

### High-Order Evaluation and Differentiation

Below: Steps to evaluate a point from the MFA. Derivatives are evaluated similarly by using the derivative of the basis function.

### Scalable Parallel Performance

Right: The MFA data model is designed for three levels of parallelism so that it can be computed efficiently on modern HPC architectures.

Below: Block parallelism with synthetic dataset partitioned into 36 blocks and modeled in parallel, blocks colored by process ID.

### Application Tests

Synthetic Analytical Functions

### Scientific Datasets

Tom Peterka, Youssef Nashed, Julian Grindeanu, and Vijay Mahadevan
Raine Yeh and Xavier Tricoche

Argonne National Laboratory
Purdue University